



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GJX
Title : Crystal Structure of the Nuclear Export Complex CRM1-Snurportin1-RanGTP
Authors : Monecke, T.; Guettler, T.; Neumann, P.; Dickmanns, A.; Goerlich, D.; Ficner, R.
Deposited on : 2009-03-09
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

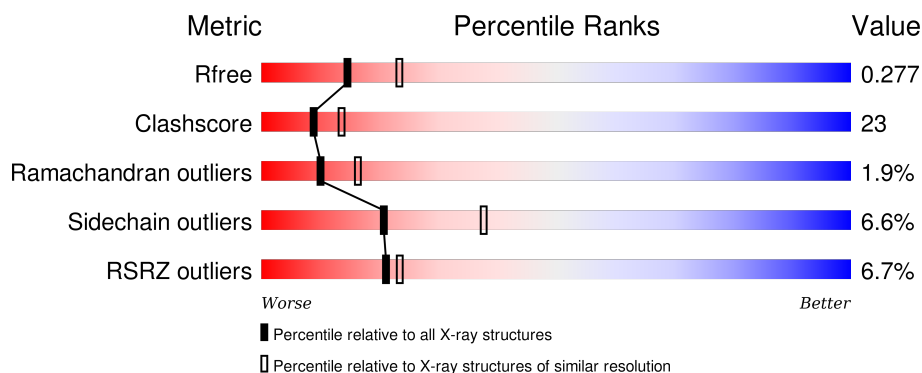
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	365	<div> <div>2%</div> <div>44% 26% 5% • 25%</div> </div>
1	E	365	<div> <div>3%</div> <div>43% 30% • 24%</div> </div>
2	C	216	<div> <div>%</div> <div>47% 28% • 21%</div> </div>
2	F	216	<div> <div></div> <div>53% 23% • 21%</div> </div>
3	A	1073	<div> <div>7%</div> <div>56% 36% 5% •</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1073	 <p>A horizontal bar chart showing the quality of chain D. The bar is divided into four segments: red (9%), green (55%), yellow (37%), and grey (1%). The segments are labeled with their respective percentages: 9%, 55%, 37%, and two small dots (• •) for the grey segment.</p>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25280 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	274	Total	C	N	O	S	0	2	0
			2222	1413	379	415	15			
1	E	279	Total	C	N	O	S	0	8	0
			2303	1466	394	427	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP O95149
B	-3	PRO	-	EXPRESSION TAG	UNP O95149
B	-2	LEU	-	EXPRESSION TAG	UNP O95149
B	-1	GLY	-	EXPRESSION TAG	UNP O95149
B	0	SER	-	EXPRESSION TAG	UNP O95149
E	-4	GLY	-	EXPRESSION TAG	UNP O95149
E	-3	PRO	-	EXPRESSION TAG	UNP O95149
E	-2	LEU	-	EXPRESSION TAG	UNP O95149
E	-1	GLY	-	EXPRESSION TAG	UNP O95149
E	0	SER	-	EXPRESSION TAG	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	1	0
			1399	910	246	238	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	ENGINEERED	UNP P62826
F	69	LEU	GLN	ENGINEERED	UNP P62826

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	5	0
			8456	5424	1421	1557	54			
3	D	1041	Total	C	N	O	S	0	8	0
			8483	5438	1427	1564	54			

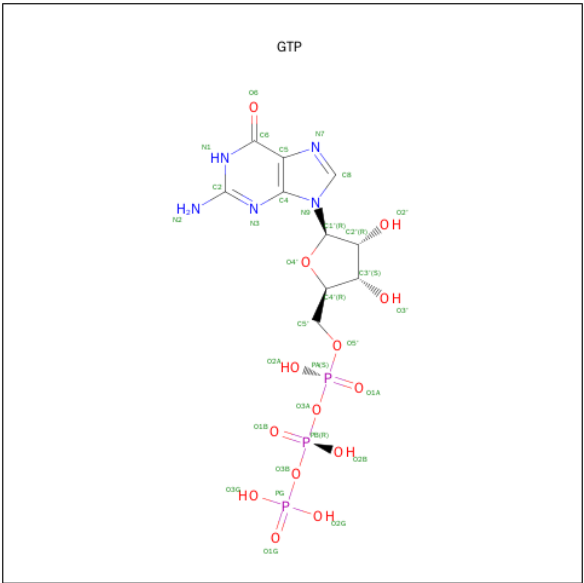
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q6P5F9
A	0	SER	-	EXPRESSION TAG	UNP Q6P5F9
D	-1	GLY	-	EXPRESSION TAG	UNP Q6P5F9
D	0	SER	-	EXPRESSION TAG	UNP Q6P5F9

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Cl	0	0
			1	1		

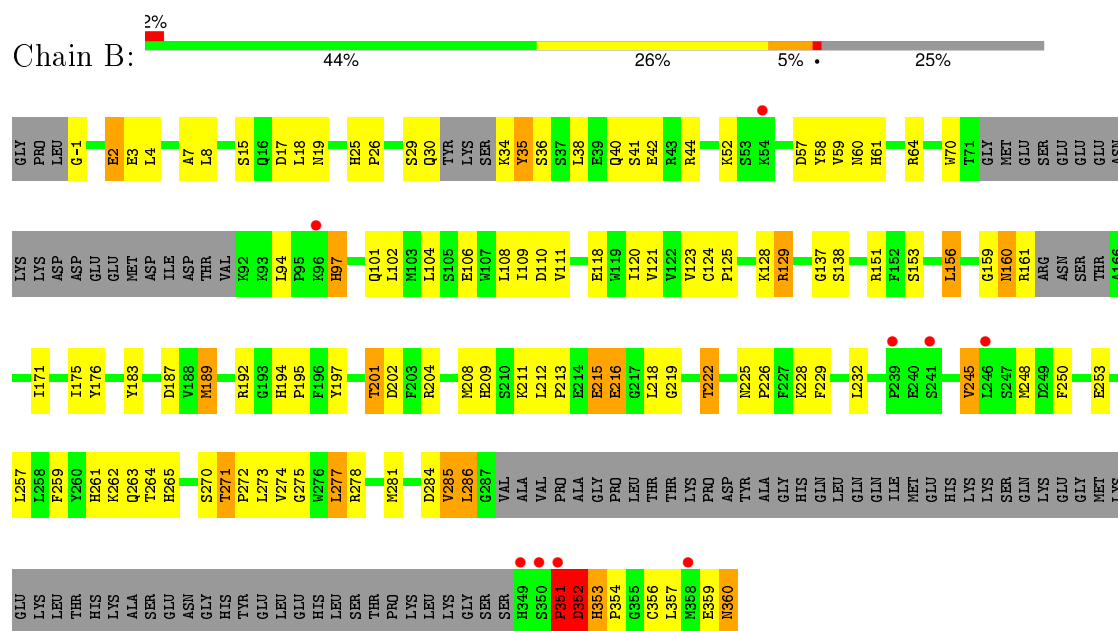
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	134	Total	O	0	0
			134	134		
8	C	58	Total	O	0	0
			58	58		
8	A	258	Total	O	0	0
			258	258		
8	E	130	Total	O	0	0
			130	130		
8	F	46	Total	O	0	0
			46	46		
8	D	333	Total	O	0	0
			333	333		

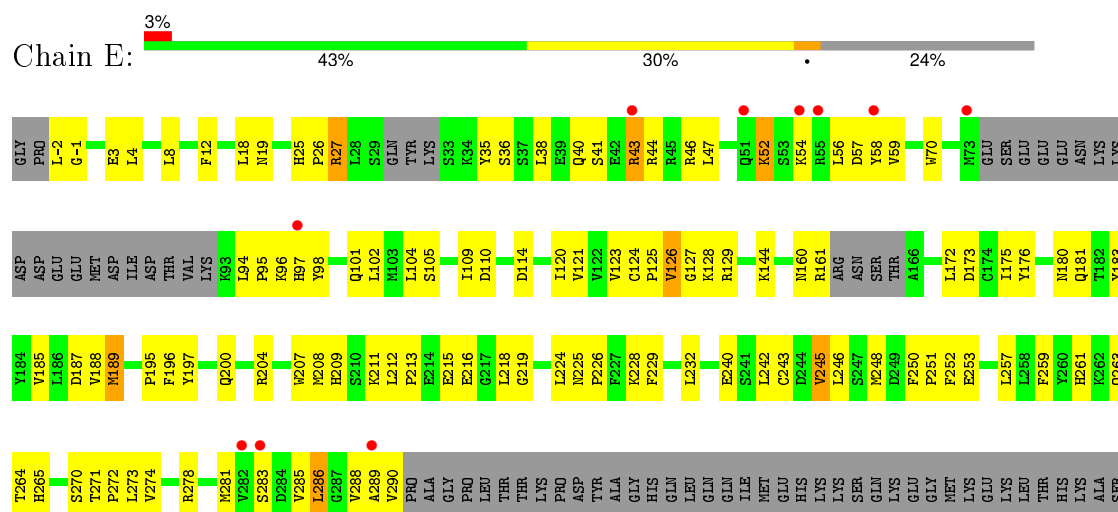
3 Residue-property plots

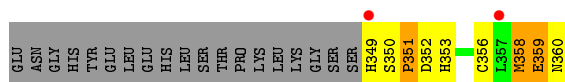
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Snurportin-1

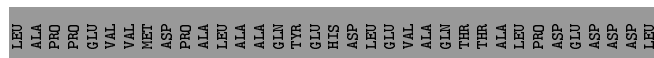
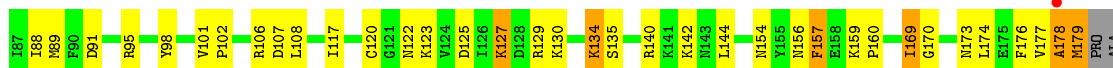


• Molecule 1: Snurportin-1

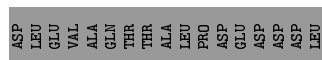




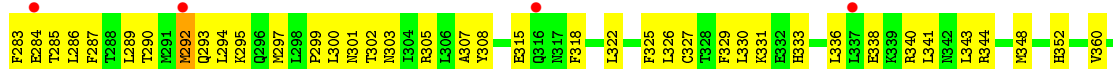
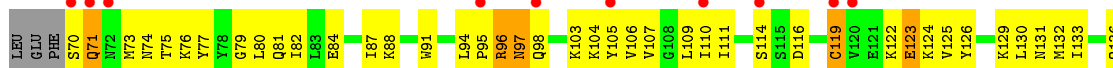
• Molecule 2: GTP-binding nuclear protein Ran

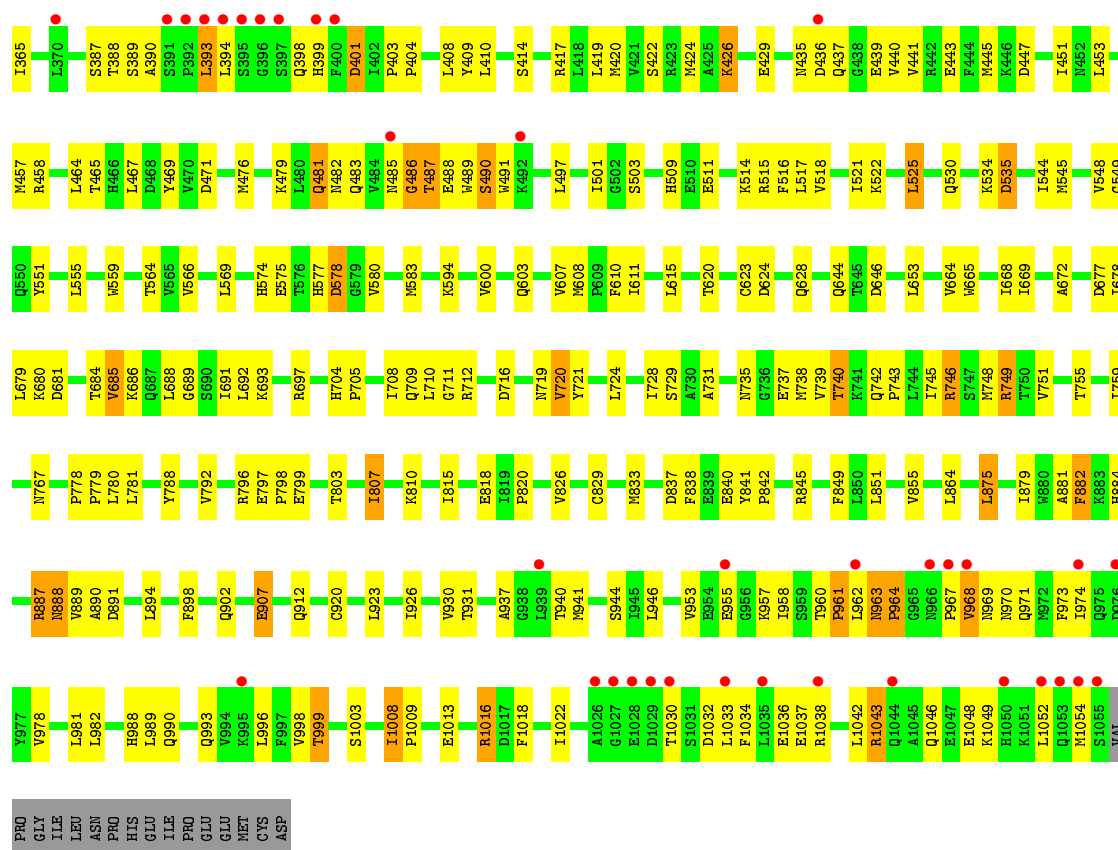


• Molecule 2: GTP-binding nuclear protein Ran

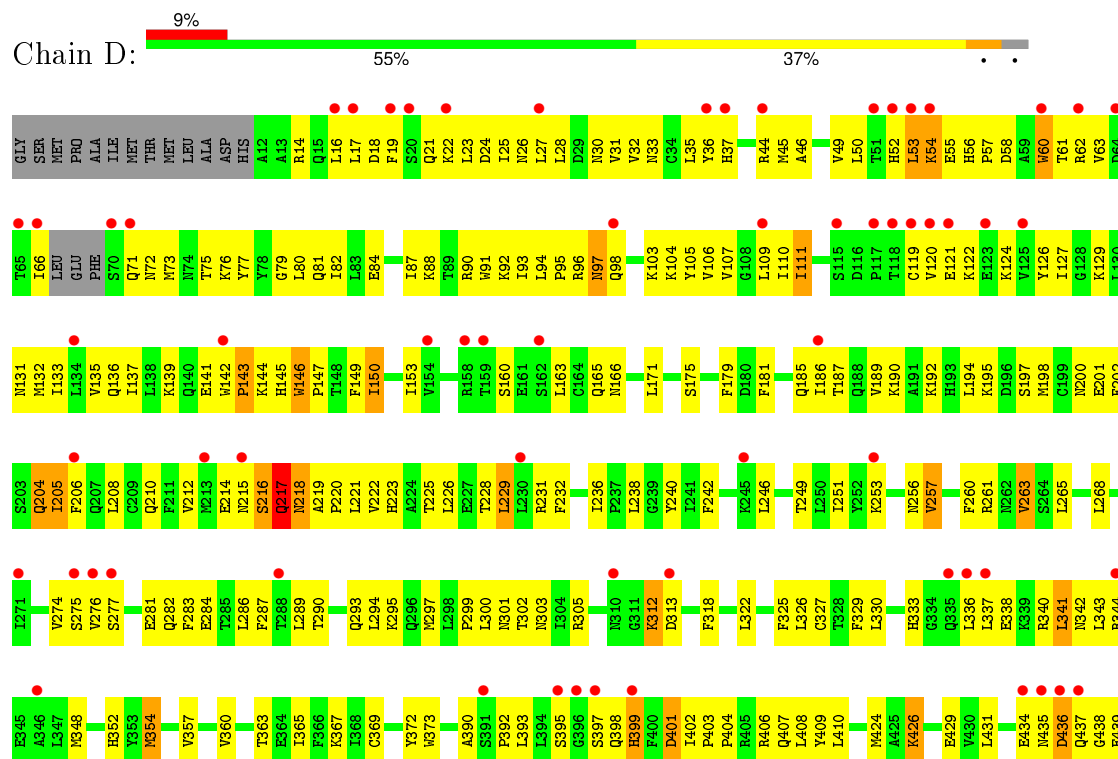


• Molecule 3: Exportin-1





• Molecule 3: Exportin-1



E1047	H970	R887	Q770	Q687	V440
E1048	Q971	R888	R771	L688	V441
K1049	H972	N889	V772	S889	M445
H1050	F973	V889	V772	E575	M445
K1051	I974	A890	V777	T576	K446
L1052	Q975	D891	V778	L691	D447
Q1053	Q975	L894	P779	L692	
H1054	V978	L894	L780	D578	
S1055			L781	G579	L453
VAL	L981	F898	L781	V580	
PRO	L982	T899	L788	M583	M457
GLY	K983	L900	V788	P705	R458
ILE		L901	V792	I591	M476
LEU	H988	Q902	V792	A592	
ASN	L989	Q912	R796	Q593	L480
PRO	Q990	Q912	L710	R597	Q481
HIS	Q993	Q916	E797	R597	M482
GLU		T917	P798	R712	Q483
ILE	L996	Y918	T803	D716	V484
PRO	F997	F919	R810	V720	M485
GLU	V998	C920	L811	Y721	G486
MET	T999	D921	L811	K722	T487
CYS		I922	I815	V607	E488
ASP	S1003	L923		M608	S490
	L1004		E818	L724	W491
	M1005	I926		F610	
		V930	Q821	O623	L497
	P1009	T931	V826	Q644	I501
	K1012	S934	C829	T645	G502
	E1013	A937	M833	D646	S503
	R1016	G938	D837	L653	E511
	D1017	L939	P838	E737	R515
	F1018	T940	E839	M738	F516
	L1019	M941	E840	V739	L517
		S944	Y841	T740	V518
	I1022	I945	P842	K741	
	F1025	L946	H843	Q742	I521
	A1026	V953	E844	P743	K522
	G1027	E954	R845	L744	L525
	E1028	E955		I745	
	D1029	E956	F849	R746	K534
	T1030	G956	L850	R749	D535
	S1031	K957	L851	Q671	
	D1032	I958	V855	V751	I544
	L1033	S959		K752	M545
	F1034	T960	L875	R753	
	L1035	P961	L875	E754	V548
	E1036	L962	I879	T755	
	E1037	N963	V880	L679	Y551
	R1038	P964	G965	K680	
		G965	V881	D681	L555
	L1042	N966	A881	S760	
	R1043	P967	F882	S764	T564
		V968	R883		V565
	Q1046	N969	H884	N767	K566

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.17Å 225.74Å 163.45Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	38.84 – 2.50 47.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.84-2.50) 86.9 (47.81-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.244 , 0.281 0.240 , 0.277	Depositor DCC
R_{free} test set	8604 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 172100 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25280	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NA, MG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.42	0/2283	0.74	3/3090 (0.1%)
1	E	0.40	0/2364	0.64	0/3202
2	C	0.34	0/1434	0.52	0/1936
2	F	0.33	0/1423	0.56	2/1921 (0.1%)
3	A	0.36	0/8628	0.51	0/11687
3	D	0.36	0/8656	0.51	0/11724
All	All	0.37	0/24788	0.55	5/33560 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PRO	CA-N-CD	-10.95	96.18	111.50
1	B	352	ASP	N-CA-C	6.65	128.97	111.00
2	F	13	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	215	GLU	N-CA-C	-5.18	97.00	111.00
2	F	13	LEU	CB-CG-CD1	5.02	119.54	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2222	0	2151	107	0
1	E	2303	0	2223	105	0
2	C	1399	0	1425	60	0
2	F	1389	0	1419	52	0
3	A	8456	0	8516	419	0
3	D	8483	0	8530	417	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	32	0	12	2	0
5	F	32	0	12	2	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	E	1	0	0	1	0
8	A	258	0	0	15	0
8	B	134	0	0	8	0
8	C	58	0	0	3	0
8	D	333	0	0	9	0
8	E	130	0	0	7	0
8	F	46	0	0	2	0
All	All	25280	0	24288	1137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.18	1.13
2:F:54:THR:HG22	2:F:176:PHE:HB3	1.19	1.11
3:D:33:ASN:HB2	3:D:44:ARG:HG3	1.33	1.09
3:A:1008:ILE:HG23	3:A:1009:PRO:HD3	1.35	1.07
1:E:350:SER:HB3	1:E:351:PRO:HD2	1.37	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	266/365 (73%)	241 (91%)	20 (8%)	5 (2%)	10	16
1	E	277/365 (76%)	253 (91%)	16 (6%)	8 (3%)	6	8
2	C	170/216 (79%)	157 (92%)	11 (6%)	2 (1%)	16	29
2	F	169/216 (78%)	157 (93%)	9 (5%)	3 (2%)	11	18
3	A	1042/1073 (97%)	945 (91%)	79 (8%)	18 (2%)	11	19
3	D	1045/1073 (97%)	952 (91%)	71 (7%)	22 (2%)	9	14
All	All	2969/3308 (90%)	2705 (91%)	206 (7%)	58 (2%)	10	15

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	216	GLU
1	B	351	PRO
2	C	169	ILE
3	A	123	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	249/327 (76%)	229 (92%)	20 (8%)	15	28
1	E	257/327 (79%)	242 (94%)	15 (6%)	25	45
2	C	151/185 (82%)	138 (91%)	13 (9%)	13	24
2	F	150/185 (81%)	139 (93%)	11 (7%)	17	32
3	A	950/973 (98%)	889 (94%)	61 (6%)	22	39
3	D	953/973 (98%)	894 (94%)	59 (6%)	23	41
All	All	2710/2970 (91%)	2531 (93%)	179 (7%)	21	38

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	746	ARG
1	E	56	LEU
3	D	821	GLN
3	A	807	ILE
3	A	999	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	969	ASN
1	E	101	GLN
3	D	853	GLN
3	A	970	ASN
3	A	1046	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	217	-	25,34,34	0.95	1 (4%)	34,54,54	1.86	8 (23%)
5	GTP	F	217	-	25,34,34	0.95	1 (4%)	34,54,54	1.85	7 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	217	-	-	0/18/38/38	0/3/3/3
5	GTP	F	217	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	217	GTP	C6-N1	2.51	1.37	1.33
5	C	217	GTP	C6-N1	2.76	1.38	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	217	GTP	N3-C2-N1	-4.63	120.39	127.44
5	F	217	GTP	N3-C2-N1	-4.46	120.65	127.44
5	C	217	GTP	PA-O3A-PB	-4.42	120.32	132.73
5	F	217	GTP	PA-O3A-PB	-4.37	120.46	132.73
5	C	217	GTP	C2'-C1'-N9	-3.84	108.43	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	217	GTP	2	0
5	F	217	GTP	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	274/365 (75%)	0.29	9 (3%) 50 55	19, 36, 78, 112	3 (1%)
1	E	279/365 (76%)	0.33	12 (4%) 39 44	19, 37, 85, 126	0
2	C	171/216 (79%)	0.28	2 (1%) 81 83	20, 43, 73, 99	0
2	F	171/216 (79%)	0.25	1 (0%) 90 91	20, 42, 77, 99	0
3	A	1041/1073 (97%)	0.50	74 (7%) 19 21	14, 46, 100, 152	1 (0%)
3	D	1041/1073 (97%)	0.60	100 (9%) 10 11	16, 46, 107, 156	5 (0%)
All	All	2977/3308 (89%)	0.47	198 (6%) 21 23	14, 43, 96, 156	9 (0%)

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	10.3
3	A	1053	GLN	9.3
3	D	967	PRO	8.3
3	D	1055	SER	8.1
3	D	19	PHE	7.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NA	B	361	1/1	0.92	0.18	0.84	34,34,34,34	0
4	NA	E	361	1/1	0.83	0.19	0.83	64,64,64,64	0
5	GTP	F	217	32/32	0.98	0.15	-0.14	14,27,40,50	0
6	MG	F	218	1/1	0.95	0.15	-0.36	33,33,33,33	0
6	MG	C	218	1/1	0.77	0.17	-0.50	40,40,40,40	0
5	GTP	C	217	32/32	0.97	0.14	-0.82	13,27,39,52	0
7	CL	E	362	1/1	0.95	0.11	-1.75	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.